Supporting Information for

Engineering Globins for Efficient Biodegradation of Malachite Green:

Two Case Studies of Myoglobin and Neuroglobin

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Table S1. Summary of data collection and refinement statistics of H64D Mb.

Wavelength	0.9791
Resolution range	24.15 - 1.6 (1.657 - 1.6)
Space group	P 21 21 21
Unit cell	39.74 49.12 77.44 90 90 90
Total reflections	261270 (27042)
Unique reflections	20632 (2037)
Multiplicity	12.7 (13.3)
Completeness (%)	99.92 (100.00)
Mean I/sigma(I)	19.84 (6.93)
Wilson B-factor	15.08
R-merge	0.09199 (0.5325)
R-meas	0.09601 (0.5538)
R-pim	0.02712 (0.151)
CC1/2	0.998 (0.964)
CC*	1 (0.991)
Reflections used in refinement	20645 (2037)
Reflections used for R-free	1020 (99)
R-work	0.1781 (0.2046)
R-free	0.1890 (0.2194)
CC(work)	0.958 (0.872)
CC(free)	0.951 (0.886)
Number of non-hydrogen atoms	1454
macromolecules	1218
ligands	43
solvent	193
Protein residues	153
RMS(bonds)	0.008
RMS(angles)	1.16
Ramachandran favored (%)	97.35
Ramachandran allowed (%)	2.65
Ramachandran outliers (%)	0.00
Rotamer outliers (%)	0.00
Clashscore	5.13
Average B-factor	19.54
macromolecules	17.88
ligands	14.89
solvent	31.02

Statistics for the highest-resolution shell are shown in parentheses.

Table S2: Docking results of MG to H64D Mb AutoDock program.

Model	$E_{binding}$ [a]	$E_{inter\text{-}mol}$ [b]	E_{vdw} [c]	E_{elec} [d]
1	-5.92	-6.82	-2.35	-0.20
2	-5.90	-6.79	-2.25	-0.19
3	-5.87	-6.77	-2.24	-0.21
4	-5.82	-6.72	-2.18	-0.21
5	-5.81	-6.70	-2.22	-0.19
6	-5.73	-6.63	-2.14	-0.21
7	-5.71	-6.60	-2.15	-0.19
8	-5.62	-6.52	-2.23	-0.21
9	-5.59	-6.48	-2.07	-0.16
10	-5.59	-6.48	-2.08	-0.22

[a] Binding energy. [b] Intermolecular energy. [c] van der Waals energies. [d] Electrostatic interactions.

Table S3. Docking results of MG to A15C/H64D Ngb AutoDock program.

Model	$E_{binding}$ [a]	$E_{inter\text{-}mol}$ [b]	E_{vdw} [c]	E_{elec} [d]
1	-5.42	-6.61	-2.40	-0.01
2	-5.38	-6.57	-2.45	-0.01
3	-5.37	-6.56	-2.45	-0.01
4	-5.34	-6.53	-2.33	0.0
5	-5.32	-6.51	-2.33	0.02
6	-5.29	-6.49	-2.40	0.0
7	-5.28	-6.47	-2.00	-0.07
8	-5.28	-6.47	-2.26	0.02
9	-5.26	-6.45	-2.34	-0.01
10	-5.23	-6.43	-2.36	0.02

[a] Binding energy. [b] Intermolecular energy. [c] van der Waals energies. [d] Electrostatic interactions.